

CAN ONE CONTROL IGNITION OF A BINARY-FUEL SPRAY?

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ABSTRACT

Evaporation and ignition of a binary-fuel cluster of drops is described by models under the assumptions that the volatile compound has infinite volatility with respect to the solvent and that the chemistries of the two compounds are independent. A Damkohler number criterion developed for use in sprays is utilized to determine the ignition time. Another criterion is used to determine the ignition location which can be either around individual drops, or around groups of drops inside the cluster, or around the entire cluster.

Results show that except for very dilute situations where the initial liquid mass fraction of the volatile is very small, ignition always occurs around the entire cluster. Otherwise, ignition occurs around groups of drops inside the cluster but never around individual drops even though the ratio of the distance between the centers of two adjacent drops by the drop diameter is greater than thirty five.

Studies performed by varying the air/fuel mass ratio for a variety of parametric combinations show that : (1) At typical gas temperatures for combustion devices, the ignition of very dense clusters of drops is strongly-controlled by solvent ignition, whereas that of very dilute clusters of drops is strongly-controlled by ignition of the volatile. In the dense and dilute regimes neither the solvent nor the volatile strongly control ignition. These conclusions are independent of the amount of volatile initially present in the liquid. (2) The concept of volatility is more closely associated with the latent heat of evaporation in the very dense regime, and more closely associated with the saturation pressure curve in the very dilute regime. (3) By increasing the ambient gas temperature one gradually gains control of ignition in the dense and dilute regimes through the solvent and volatile respectively, (4) The initial slip velocity between phases affects ignition only in the very dilute regime. (5) Changes in the cluster size affect the ignition time only in the very dense regime. (6) The previous conclusions are valid under the assumption of identical kinetics for the two compounds. When different kinetics is considered, it turns out that kinetic effects overwhelmingly dominate ignition.

INTRODUCTION

The majority of practical fuels used either in power plants or for propulsion are multicomponent fuels. Since they are composed of several chemical species, the interaction among the various characteristics of the pure chemical components determines the characteristics of the fuels in terms of evaporation, ignition and combustion.

Since many of these multicomponent fuels contain tens and sometimes more than a hundred pure components, it is found convenient to categorize these components according to a criterion which is thermodynamically not well defined, but which is practically useful; this is the concept of volatility. Volatility is, a priori, thermodynamically related both to the latent heat of evaporation and to the saturation vapor pressure curve versus the temperature. Using the concept of volatility, the multitude of chemical components is partitioned into two components: the ~~solute~~^{vent} and the volatile. The ~~solute~~^{vent} contains the heavier, more viscous components which evaporate slowly. "The volatile contains the lighter, less viscous components which evaporate rapidly. When these criteria are used to define ~~solute~~^{vent} and volatile respectively, it turns out that the concept of volatility is more closely related to the saturation vapor pressure curve versus the temperature in the very dilute region of the spray, and more closely related to the latent heat of evaporation in the very dense region of the spray as will be shown in this paper.

Single droplets of multicomponent fuels have been studied extensively in the past (Law et al., 1997; Sirignano and Law, 1978; Lara-Urbaneja and Sirignano, 1981; Law, 1986; Randolph et al., 1986; Aggarwal, 1989; Mawid and Aggarwal, 1990). It was found that isolated drop evaporation in a convective flow is dominated by liquid mass diffusion (Law et al., 1977; Sirignano and Law, 1978; Lara-Urbaneja and Sirignano, 1981; Law, 1986; Randolph et al.,

1986) due to the creation of Hill vortices inside the drops through the intermediary of the shear layer which forms at the drop surface as a result of the slip velocity between phases. The internal convection thus established enhances liquid mass diffusion, which is otherwise a very slow process, to the point that liquid mass diffusion of the volatile becomes a controlling process during evaporation. Studies of isolated drop ignition (Aggarwal, 1989; Mawid and Aggarwal, 1990) understandably identified the volatile as the component initiating ignition, and it was found that the addition of a small amount of volatile enhances ignition considerably (Mawid and Aggarwal, 1990). Mawid and Aggarwal (1990) acknowledge that their study is only valid in the dilute limit; an indication of this restriction is the fact that they find ignition to be dominated by individual drop ignition rather than by group - drop ignition. In contrast, experimental observations of burning sprays (Allen and Hanson, 1986a; Allen and Hanson, 1986b; Mizutani et al., 1993; McDonnell et al., 1992; McDonnell et al., 1993; Rudoff et al., 1989; Mao et al., 1985) show multiple flames, each flame surrounding a group of drops. Individual drop ignition with flames quickly merging and surrounding groups of drops is still possible; however, it has not been experimentally observed.

A more recent study of clusters of drops (Harstad and Bellan, 1991) portraying the groups of drops identified experimentally both in burning (Allen and Hanson, 1986a; Allen and Hanson, 1986b; Mizutani et al., 1993; McDonnell et al., 1992) and non burning sprays (McDonnell et al., 1992; McDonnell et al., submitted; Rudoff et al., 1989; Mao et al., 1985) has revealed a different physical picture than that emerging from the isolated drop studies. The results showed that there are two processes which may influence evaporation of the volatile. The first process is the liquid mass diffusion already identified by the isolated drop studies. The second process

is surface layer stripping which is the removal of the volatile at the rate of evaporation of the ^{volatile} solute.

For dense clusters of drops the slip velocity between drops and gas relaxes very fast (Harstad and Bellan, 1991; Bellan and Harstad, 1981a) because the cluster exposes a large area to the flow (there are many drops per unit area). Thus, there is no time to establish a shear layer at the drop surface, and as a consequence internal drop circulation through the Hill vortex does not occur. The result is that liquid mass diffusion remains a slow process with a characteristic time larger than the drop lifetime, and thus cannot influence evaporation of the volatile. The mass fraction of the volatile within the drop stays frozen in time, and the volatile leaves the surface at the same rate as the ^{volatile} solute; this is surface layer stripping. Experiments performed in low pressures so as to suppress buoyancy (Randolph et al., 1986) have shown precisely this type of behavior: the mass fraction of the volatile stays frozen in time and the volatile leaves the surface at the rate of evaporation of the ^{volatile} solute.

For dilute clusters of drops it was found (Harstad and Bellan, 1991) that the slip velocity between phases relaxes in a time comparable to the lifetime of the drop, and thus both liquid mass diffusion and surface layer stripping are important. The parameter characterizing the relative importance of these two phenomena, Be , is the ratio of the mass regression rate to a characteristic volatile diffusion rate (Harstad and Bellan, 1991). If $Be \ll 1$, then diffusion into the drop boundary layer (determines the rate of species transfer from the liquid core to the drop surface and liquid mass diffusion is important. If $Be \gg 1$, then surface layer stripping is important. Plots of Be versus the residual drop radius show that for initially dense clusters of drops $Be \gg 1$ during the drop lifetime (after adjustment from the initial condition). In

contrast, for initially dilute sprays $Be = [O(1) - O(10)]$ during the drop lifetime (after adjustment from the initial condition).

On the basis of this behavior it has been possible to classify clusters of drops according to the value of the nondimensional radius of the sphere of influence around each drop. For monodisperse clusters, the nondimensional radius of the sphere of influence is defined as the ratio of the distance between the centers of two adjacent drops divided by the drop diameter. When this ratio has a value smaller than 10, the cluster is very dense. When this ratio has a value between 10 and 15, the cluster is dense. Dilute clusters are those for which the value of the radius of the sphere of influence is larger than 15 but smaller than 30. Very dilute clusters are those for which the nondimensional radius of the sphere of influence is larger than 30. The drops in very dilute clusters behave as if they were isolated from each other.

The present study addresses ignition of clusters of binary - fuel drops composed of a solute and a volatile as discussed above. The model for drop evaporation is that of Harstad and Bellan, 1991 and it is briefly recalled in the next section. The ignition model is described in the next section as well. Results are obtained for a variety of fuel combinations and an extensive parametric study is performed. It is shown that when the kinetic parameters are identical for the two components it is only in the very dilute regime that ignition is governed by the evaporation of the volatile; this is a situation which does not have practical interest since spray ignition is desirable well before the spray becomes dilute. It is also shown that, for the same kinetic parameters, in the very dense regime ignition is controlled by the solute. Interestingly, for identical kinetic parameters and at a typical gas temperature in the near field of the atomizer in combustion devices, ignition cannot be controlled in the dense or dilute regimes because neither

solvent nor volatile are strongly dominating ignition. Departures from these conclusions are shown to occur when some parameters are varied.

PHYSICAL CONFIGURATION AND MODEL

1. The evaporation model.

The physical configuration studied here is exactly the same as in Harstad and Bellan, 1991, but whereas in that investigation it is only evaporation that was studied, here ignition may occur as well. As will be discussed below, ignition of a multicomponent fuel is an intricate chemical problem which has not yet received the interest that it deserves because of the lack of precise chemical kinetic information regarding even single-component fuels.

Following the configuration described in Harstad and Bellan, 1991, in the present study, a cluster composed of binary-fuel, monodisperse drops moves in an ambient gas with a velocity u_d which is measured with respect to a coordinate system fixed with respect to the ambient. The cluster is assumed to be spatially homogeneous in thermodynamic quantities on a length scale of the order of many drop radii. Initially the gas inside the cluster is quiescent, and so is the gas in the ambient. However, once the drops start moving, the gas inside the cluster acquires a velocity, u_g . Thus, the axial slip velocity between drops and gas inside the cluster is $u_{sl,a} = u_d - u_g$.

Since the temperature of the ambient is much larger than the initial drop temperature, the drops heat up, evaporate and might ignite. The pressure inside the cluster is atmospheric and constant, so that the change in the gas temperature inside the cluster implies a change in the volume of the cluster. The boundary of the cluster is by definition the envelope of the drops

which moves with a velocity dR_{cl}/dt with respect to the cluster center, '1'bus, the drops have not only an axial velocity with respect to the gas, but also a radial velocity. The motion of the drops is assumed to be self-similar, so that drops occupy positions $r = \xi R_{cl}$, where R_{cl} is the cluster radius and ξ is fixed for a given drop; $0 < \xi < 1$. With this definition, the relative radial motion for a drop interior to the cluster is $\xi(dR_{cl}/dt - u_{ge})$ where u_{ge} is the gas radial motion at the cluster edge, The relative radial motion of a drop at the cluster edge is $u_{re} = dR_{cl}/dt - u_{ge}$. The dynamics of the drops has been described in detail elsewhere (Bellan and Harstad, 1990; Harstad and Bellan, 1989; Bellan and Harstad, 1987b) and thus will not be repeated here. Of special interest is the fact that the drag force depends upon the drop number density, the blowing of mass from the drops as they evaporate (which depends itself upon the drop number density), and the slip velocity inside the cluster.

The binary fuel is assumed to be composed of a ~~solute~~^{vent} and a volatile whose volatility is much larger than that of the ~~solute~~^{vent}; practically, the volatility of the solute is infinite with respect to that of the ~~volatile~~^{solvent} (Harstad and Bellan, 1991). Each drop is composed of a liquid core whose motion is described by the Hill vortex solution, and a thin boundary layer at the drop surface. The evaporation model is described in detail in Harstad and Bellan, 1991. The highlight of the model is the definition of a nondimensional quantity, Be , which represents the ratio of the drop mass regression rate to a characteristic volatile cliff ision rate. As discussed above, when $Be \ll 1$, diffusion into the drop boundary layer governs the rate of volatile species transfer from the liquid core to the drop surface and evaporation from the surface occur-s at a rate defined by the Langmuir - Knudsen evaporation law. In fact it is the slower of these two rates which governs evaporation since the two processes are sequential. When $Be \gg 1$, the transfer of

volatile from the liquid core to the gas phase is governed by surface layer stripping, that is by the regression rate of the drop (Harstad and Bellan, 1991). Because $Be \gg 1$ for drops in dense clusters, whereas $Be = [O(1) - O(10)]$ for drops in dilute clusters (Harstad and Bellan, 1991), a qualitatively different process is found to control evaporation of the volatile in these two regimes.

2. The ignition model.

Ignition is modeled under the assumption that the chemistry of the ~~solute~~^{vent} and that of the volatile are independent. This assumption is not realistic for hydrocarbons which decompose into simpler compounds who ultimately interact chemically. However, given the lack of knowledge of the detailed chemistry for hydrocarbons more complicated than propane, any other assumption would be equally unrealistic and would additionally introduce an unwarranted degree of complexity.

Under the above assumption, one can define two independent Damkohler numbers, one for the ~~solute~~^{vent} and one for the volatile as follows:

Y_{oa} if oxygen-rich

$$Da_s = \frac{\theta_{ga}^2}{\theta_{r,s}^2} \frac{C_{pg}}{\lambda'_{gW_o}} \left(\frac{R^o p C_{pg} \bar{W}_s}{R_u C_s} \right)^2 R_2^4 C^{-2} \exp \left(\frac{\theta_{r,s}}{\theta_{ga}} \right) \quad (1)$$

$Y_{Fva,s} \phi'_{s,s}$ if
oxygen-lean

Y_{oa} if oxygen-rich

$$Da_v = \frac{\theta_{ga}^2}{\theta_{r,v}^2} \frac{C_{pg}}{\lambda'_{gW_o}} \left(\frac{R^o p C_{pg} \bar{W}_v}{R_u C_v} \right)^2 R_2^4 C^{-2} \exp \left(\frac{-\theta_{r,v}}{\theta_{ga}} \right) \quad (2)$$

$Y_{Fva,v} \phi'_{s,v}$ if
oxygen-lean

The symbols are all explained in the Nomenclature.

These Damkohler numbers are a measure of the importance of chemical rates with respect to the diffusion rates, and have been used in the past to determine ignition of clusters of drops (Bellan and Harstad, 1990; Law and Chung, 1980). According to Law and Chung, 1980, ignition of a drop in a reactive environment will occur if the Damkohler number is larger than the ignition Damkohler number. The ignition Damkohler number is found (Law and Chung, 1980) using large activation energy asymptotic in the quasi-steady gas phase equations for a single drop in surroundings where fuel vapor may be present. For a binary fuel, the ignition Damkohler numbers for ^{volatile} solute and volatile are respectively obtained as explained in Bellan and

Harstad, 1987b. For an oxygen-lean mixture, the correlation of Law and Chung, 1980 is used for Da_{ign} versus κ for $1 < \kappa < 10^3$. For oxygen-rich mixtures, the results presented in curve form by Law and Chung [19] for $0 < \gamma < 10^3$ and $0.005 < \beta < 1$ are recorrelated by including values of Da_{ign} for $\gamma > 10^3$ and values of $\beta < 0.005$; these values are obtained by using asymptotic limits and matching by continuity.

Thus, ignition will be initiated by the ^{volatile} solvent if

$$Da_s \geq Da_{s,ign} \quad (3)$$

and ignition will be initiated by the volatile if

$$Da_v \geq Da_{v,ign} \quad (4)$$

When neither of these inequalities is satisfied during evaporation, the cluster of drops does not ignite. Limiting cases are ignition of drops just after they have completely evaporated, in which case $R_1 = 0.05$, or ignition of drops just as they have been introduced into the hot environment, in which case R_1 is very close to unity.

The model developed by Bellan and Harstad, 1987b not only predicted the timing of ignition, but also predicted whether ignition occurs around isolated drops in a spray, around clusters of drops, or inside clusters of drops but around a few of the drops rather than around the entire cluster. The criteria previously developed will be used here as well in order to determine the location of ignition.

RESULTS AND DISCUSSION

As mentioned above, the consensus from isolated drop studies is that ignition of binary - fuel

drops is dominated by ignition of the volatile, and thus that by adding a small amount of volatile, ignition can be considerably enhanced. One of the goals of this study is to ascertain if this conclusion can be extended to a real spray which contains clusters of drops of various equivalence ratios, and thus of various number densities.

1. Typical behavior.

For the baseline set of solutions the ~~solvent~~^{vent} was chosen to be No. 2 GT fuel oil (light Diesel oil) and the volatile was chosen to be n-decane. The initial values of the dependent variables are $u_d^0 = 200$ cm/s, $R_{cl}^0 = 3$ cm, $R_d^0 = 2 \times 10^{-3}$ cm, $T_{ga}^0 = 1000$ K, $T_{gs}^0 = 350$ K, $p = 1$ atm, $Y_{Fva}^0 = 0$, $Y_{HV,c}^0 = 2 \times 10^{-2}$. The properties of the two compounds are listed in Harstad and Bellan, 1991, and the vapor pressure curves are presented there as well. The ignition chemical kinetic parameters were here chosen to be identical for the two compounds: $A_{ign} = 3.8 \times 10^{11}$ cm³/(mole-s), and $E_{ign} = 30$ kcal/mole (Harstad and Bellan, 1991; Bellan and Harstad, 1987 b). Calculations were performed for an extended range of air/fuel mass ratios from 0.314 to over 25 (the stoichiometric value is 15) corresponding to a nondimensional radius of the sphere of influence of 8.4 to 37, thus encompassing the very dense, dense, dilute and very dilute regimes according to the definition given in Harstad and Bellan, 1991.

The results show that for these initial conditions clusters having $\Phi^0 = 0.314$ do not ignite, whereas clusters having $\Phi^0 = 0.785$ ignite at the time when the drops have completely evaporated (chosen to correspond to $R_1 = 0.05$). At the other extreme, for $\Phi^0 = 25$ the drops ignite at $R_1 = 0.98$, which is practically when they are introduced into the hot ambient. The ignition location is always outside the cluster, except for values of Φ^0 larger than 34, where ignition is found to occur inside the cluster at locations such that the resulting flame surrounds

groups of drops. In all following calculations discussed in this paper, ignition occurred around clusters of drops. Figure 1 shows the ignition time, t_{ign} , versus R_2^0 , whereas Fig. 2 shows both t_{ign} and $R_{1,\text{ign}}$ versus Φ^0 . On the plots depicted in these figures, a distinction is made between situations when ignition occurs due to the solvent, and when ignition is due to the volatile.

The very dense regime is dominated by solvent ignition, whereas the very dilute regime is dominated by volatile ignition in agreement with the results of previous studies of isolated drops. These results are not surprising since it has been previously found (Harstad and Bellan, 1991) that evaporation is dominated by the solvent in the very dense regime whereas it is dominated by the volatile in the very dilute regime. Surprisingly, between these two extreme regimes ignition seems to be sometimes initiated by the volatile and sometimes by the solvent. The previous study of binary-fuel drop evaporation in clusters (Harstad and Bellan, 1991) does not provide an explanation to this surprising behavior.

In order to explain the behavior in the dense and dilute regimes, another set of calculations were performed where $A_{\text{ign},s}$ was taken negative if in the initial calculations it was found that the solvent was initiating ignition, and $A_{\text{ign},v}$ was taken negative if in the initial calculations it was found that the volatile was initiating ignition. Thus, ignition of the initiating compound was “turned off” in order to see if the other compound would ignite the cluster; and if ignition occurred, the important consideration was to quantify the change in t_{ign} and $R_{1,\text{ign}}$. Results from these calculations show that in the very dense regime ignition does not occur at all, thus confirming the conclusion that ignition is strongly controlled by the solvent. In the very dilute regime, physically incorrect results are obtained where γ becomes negative; this confirms the conclusion that it is the volatile which strongly controls ignition in the very dilute regime.

Between these two regimes, ignition is obtained at about the same t_{ign} and $R_{1,\text{ign}}$ as with the original calculations; the ratio of t_{ign} and $R_{1,\text{ign}}$ with the values obtained in the original calculations is at most 1 %. This proves that it is neither the solvent nor the volatile which controls ignition in these intermediary regimes, and that it is only the details of the calculation which decide upon the compound initiating ignition. Since these details can never be modeled in a totally accurate manner, it is impossible to identify the compound initiating ignition in these intermediary regimes.

Since solvent-controlled or volatile-controlled evaporation has been associated with the value of Be , it is instructive to think again in terms of processes occurring at different characteristic times. Here there are two competing processes determining the compound initiating ignition: the relaxation rate of the slip velocity and the rate at which the Damkohler number approaches the ignition Damkohler number for either one of the compounds. If the rate at which the Damkohler number approaches the ignition Damkohler number is much slower than the relaxation rate of the slip velocity, then Be becomes very large by the time ignition occurs and thus the solvent controls ignition. In contrast, if ignition occurs very fast with respect to the relaxation rate of the slip velocity, then Be remains relatively small and the volatile controls ignition. Plots of the slip velocity versus t and of Be versus t can be found respectively in Figs. 3 and 4 corroborating the above interpretation.

The practical conclusion from these results is that in realistic spray situations where the system has been optimized for maximum efficiency, one should never plan to control ignition by increasing the amount of volatile in the fuel. This is because the volatile strongly controls ignition only in the very dilute part of a spray, well past the point of efficient operation. Since

usually it is the volatile which is the most expensive part of the fuel, this conclusion is important in reducing energy costs associated with using additional amounts of volatile in binary fuels. Rather than changing the composition of the fuel, it will be shown below that by changing the regime of operation, ignition can be made to be strongly controlled by the solvent in part of the dense regime adjacent to the very dense regime, and that the volatile can be made to strongly control ignition in parts of the dilute regime. Thus, at fixed composition one may control ignition using the solvent or the volatile by changing the surroundings of the spray.

2. Effect of the initial amount of volatile in the liquid.

Calculations were performed by increasing $Y_{HV,c}^0$ from 0.02 to 0.05 and 0.2. The results show identical values for t_{ign} and $R_{l,ign}$ in the very dense regime, in agreement with the conclusion that the volatile does not control ignition in this regime. In the very dilute regime, small changes were observed for both t_{ign} and $R_{l,ign}$, however, for these larger values of $Y_{HV,c}^0$ ignition occurs around the entire cluster rather than around groups of drops inside the cluster. For these larger amounts of volatile the amount of volatile vapor is correspondingly larger, and this stronger flux pushes the ignition location outside the cluster. The situation is similar to that of the flame motion for isolated drop evaporation: a stronger mass flux pushes the flame further away from the drop.

3. Effect of the volatile identity.

Calculations were performed by replacing n-decane by n-hexane and also by n-heptane. Both compounds have a larger latent heat than n-decane (more difficult to evaporate) and a higher saturation pressure (easier to evaporate). N-hexane has a larger latent heat than n-heptane and a higher saturation pressure than n-heptane. In all calculations $Y_{HV,c}^0 = 0.2$.

Results show negligible differences among the values for t_{ign} and $R_{1,\text{ign}}$ for all these runs. Obviously, in the very dense regime no differences are expected since the volatile is not controlling. What the results indicate is that in the very dilute regime the effect of the latent heat balances that of the saturation pressure, yielding no noticeable effect of the volatile. Note that in the model it is assumed that the volatility of the volatile is infinite with respect to that of the solvent, however differences among volatile properties are taken into account, so that if there were any noticeable effect of the volatile it would have been indicated in the results.

4. Effect of the solvent identity.

In order to explore the influence of the solvent, No. 2GT was replaced by n-decane and the volatile was chosen to be n-hexane. N-decane has a larger latent heat than No. 2GT oil and a larger saturation pressure. The results show substantial differences between the behavior of the two binary fuels.

In the very dense regime, ignition no longer occurs for clusters having $\Phi^0 = 0.785$. This indicates that the effect of the latent heat dominates that of the saturation pressure when the drops are in very close proximity. This is easy to understand since for dense clusters evaporation is limited by the availability of heat to the drops. The larger latent heat exacerbates the situation further, and prevents ignition. In the dense regime, the larger latent heat delays ignition as shown in Fig. 5 where t_{ign} and $R_{1,\text{ign}}$ are plotted versus Φ^0 . Our interpretation of the results is confirmed by the much larger value of Be at fixed Φ^0 in the dense regime. Accordingly, when the solvent is n-decane instead of No. 2GT oil, the range of strongly solvent-controlled ignition extends to larger values of R_2^0 . This is because, as explained above, for a given Φ^0 in this range, a cluster has stronger dense characteristics since I_1 is larger.

In the very dilute regime the behavior of the binary fuel is exactly the opposite to that in the very dense and dense regimes: here ignition occurs earlier in time because it is promoted by the larger saturation pressure. The evaporation of dilute clusters of drops is not limited by drop heating because the drops behave as if they were isolated, and instead it is the saturation pressure which determines volatility. Although ignition occurs earlier in time, it occurs later in the relative drop lifetime (indicated by the value of R_1) because evaporation is faster due to the higher saturation pressure.

The ignition behavior in the dilute regime combines both effects of the latent heat and the saturation pressure. As a result, ignition is sometimes promoted and sometimes hindered as clearly seen in Fig. 5 .

5. Effect of the ambient temperature.

Decreasing the ambient temperature to 800K suppresses ignition in the very dense regime and delays ignition in all other regimes as shown in the plots of Fig. 6. The results show not only a loss of the strongly solvent-controlled ignition regime, but also a much milder control of the volatile in the very dilute regime. This is the consequence of a much slower evaporation which allows enough time for the relaxation of the slip velocity, yielding values of Be larger by at least one order of magnitude in the very dilute regime. Since $Be \approx O(10)$ as illustrated in Fig. 7, both liquid mass diffusion and surface layer stripping are important. Thus, decreasing the ambient temperature not only suppresses ignition in the very dense regime and delays ignition for all Φ^0 's, but also results in a loss of control over ignition by either one of the two components. Therefore, at low ambient temperatures, ignition cannot be controlled in any regime by using the chemical constituents of the fuel.

A larger ambient temperature (1200K compared with 1000K) considerably enhances ignition to the point that ignition now occurs for smaller values of Φ^0 (for example 0.314 for which $R_2^0 = 8.9$). The strongly solvent-controlled regime extends both toward smaller and larger values of Φ^0 than in the typical case. The larger ambient temperature affects ignition in the dilute regime as well, resulting in immediate ignition for clusters having $R_{2c}^0 = 24.4$. The much shorter evaporation time does not allow relaxation of the slip velocity, and thus now the volatile strongly controls ignition in the dilute regime. Depicted in Fig. 6 are t_{ign} and $R_{1,ign}$ versus Φ^0 , and plots of Be for selected values for Φ^0 appear in Fig. 8. The very dilute regime is not considered here since calculations are stopped in the Φ^0 domain (Φ^0 is no longer increased) as soon as ignition occurs instantaneously after introduction of the cluster into the ambient. The conclusion is that at higher temperature it is easier to control ignition over a wider range of Φ^0 's, either using the solvent in the very dense and dense regimes, or using the volatile in the dilute regime. Since sprays contain clusters of drops having initially a range of air/fuel mass ratios, this means that ignition control of the *entire spray* can be achieved at high temperatures by using the chemical components of the fuel as drivers.

6. Effect of the chemical kinetics of ignition.

All the results obtained so far have contained the assumption that the ignition kinetic parameters of solvent and volatile are identical. Results from calculations where $E_{ign,s}$ has been increased by 3 % show that ignition is suppressed in the very dense regime, whereas in all other regimes there are only minor changes with respect to the baseline results (now there is an apparent domination of the volatile for the entire range of Φ^0 's, except in a very narrow range in the dense regime). Thus, a small change in the activation energy of ignition results in loss of

the strongly solvent-controlled ignition regime,

A 3% increase in $E_{\text{ign},v}$ does not produce any changes in the results obtained in the very dense regime, however ignition does no longer occur in the very dilute regime. This is an additional indication that the volatile strongly controls ignition in the very dilute regime. For all other values of Φ^0 , there is an apparent solvent dominated ignition. Similar to the conclusion when changing $E_{\text{ign},s}$, now it is the control of the volatile which is lost.

This study thus shows that the ignition kinetics has an overwhelming effect on ignition, overshadowing all other parameters. For this reason, it is recognized that no definitive results can be obtained in this investigation until the values of the chemical kinetic parameters are better known.

7. Effect of the initial slip velocity.

It is here recalled that since the gas in the cluster is initially at rest, the initial slip velocity is the initial velocity of the drops. Reducing the initial slip velocity to 100 cm/s from the typical value of 200 cm/s, results in a decrease in the evaporation rate, and this generally slightly increases the ignition time, without much change in the value of $R_{l,\text{ign}}$. In the very dense regime where evaporation is hindered by drop proximity, the lowering of u_d^0 suppresses ignition. The smaller evaporation rate in the dense regime allows relaxation of the slip velocity, resulting again in solvent strongly-controlled ignition. The change in the initial slip velocity affects the dense regime much less than the very dilute regime since in the dense regime the relaxation of the slip velocity is faster. In the very dilute regime the evaporation rate and the slip velocity relaxation rate are still comparable, so that ignition is still strongly-controlled by the volatile.

Thus the solvent strongly-controlled ignition regime moves into the dense regime whereas volatile strongly-controlled ignition remains in the very dilute regime.

8. Effect of the cluster initial radius.

When the initial radius of the cluster is decreased to be 1 cm instead of the baseline value of 3 cm, the surface/volume ratio increases accordingly. This enhances heat transfer processes from the ambient to the cluster. Heat transfer processes are very important in the dense regime, but are unimportant in the dilute regime where evaporation is not limited by the amount of heat available for each drop. As a result, ignition is now obtained for smaller values of Φ^0 (denser clusters) than in the corresponding calculation with the larger initial cluster radius as can be seen in Fig. 9. The solvent strongly-controlled ignition regime moves accordingly toward the smaller Φ^0 's; this is also confirmed by plots of Be versus R_1 shown in Fig. 10. The very dilute regime is unaffected by the change in the initial cluster radius, as discussed above.

SUMMARY AND CONCLUSIONS

A model of binary-fuel drop evaporation in clusters has been used in conjunction with an ignition model based upon the Damkohler number criterion for drops in sprays to study ignition of clusters of drops. The assumption is also made that the chemistry of the two compounds is independent from each other.

Calculations were performed by varying the air/fuel mass ratio for different values of the main parameters. Small values of the air/fuel mass ratio correspond to very dense clusters of drops, whereas large values of the air/fuel mass ratio correspond to very dilute clusters of drops in which there is no drop interaction. Baseline results show that in a typical near-field-atomizer

gas temperature, ignition is strongly controlled by the solvent in the very dense cluster regime, and that ignition is strongly controlled by the volatile in the very dilute regime, In the intermediary dense and dilute regimes, control by either one of the compounds is very weak and depends entirely upon the details of the calculation. '1'bus, the isolated drop results are recovered in the very dilute regime, however it is found that it is qualitatively a different process which controls ignition in a real spray, The practical conclusion is that at typical near-field-atomizer gas temperatures it is useless to use more expensive fuels having larger amounts of volatile for the purpose of enhancing ignition because it is only the very dilute clusters of drops which will benefit from this treatment. These clusters of drops appear only at relatively large distances from the atomizer and thus do not participate in the ignition process.

As the ambient temperature of the gas is increased, it is easier to gain control of ignition over a larger range of air/fuel mass ratios. This is achieved by using the volatile in the very dilute and increasingly in the dilute regime, and by using the solvent in the very dense and increasingly in the dense regime. Eventually, a temperature is reached at which ignition control of the entire spray can be achieved through ignition control of clusters at all air/fuel mass ratios.

Studies of the effect of the compound used as solvent revealed that the concept of volatility is associated more with the latent heat of evaporation in the very dense cluster regime and is associated more with the saturation pressure in the very dilute cluster regime.

It is also shown that variations of the initial slip velocity between phases affect the results only in the very dilute regime because of the short relaxation time of the slip velocity in the very dense regime. In contrast, changes in the size of the cluster affect the ignition timing only in the very dense regime which is limited by the amount of heat available to each drop to increase its

temperature and evaporate.

For very low values of the initial amount of volatile in the liquid, ignition in the very dilute regime is found to occur around groups of drops inside the cluster. For air/fuel mass ratios outside the very dilute regime, ignition occurs around the entire cluster of drops. As the initial amount of volatile in the liquid is increased, it is found that ignition occurs exclusively around the entire cluster.

All of the above results were found under the assumption that the chemical kinetic parameters of the two compounds were identical. Studies of the effect of the chemical kinetic parameters show that these have an overwhelming effect on the ignition results. Solvent-controlled ignition can be lost when the solvent activation energy is slightly increased. Equivalently, volatile-controlled ignition can be lost when the volatile activation energy is slightly increased. Since chemical kinetic parameters of hydrocarbons are not known for hydrocarbons more complicated than propane, definitive conclusions must await precise chemical kinetic information.

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